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Greg Ruderman, "A Microforce-Based Theory for Energetic Materials"
JANNAF Abstract

(Statement A)

A Microforce-Based Theory for Energetic Materials

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Abstract

Thermomechanical modeling of energetic materials such as solid rocket motor propellants and explosives is an extremely complex problem due to the large number of behaviors such a material may exhibit. Experiments have shown that these materials may be nonlinearly viscoelastic and may also exhibit plastic flow, phase changes, and combustion. In addition, these phenomena are often strongly coupled, making empirically based modeling very difficult.

Employing advanced tools of continuum thermomechnanics, we have developed a fully three-dimensional framework, which in its most general form is able to model all the mentioned behaviors of energetic materials. The concept of microforces, forces that drive changes in material microstructure, is employed to generate consistent equations of evolution for combustion and phase transitions. The method of generating equations for thermomechanical behavior using microforces begins with the generation of a free-energy function that encompasses all the material changes. The Clausius-Duhem inequality, a statement of the second law of thermodynamics, is then applied, restricting the material behavior to be thermodynamically correct *a priori*. Appropriate forms of coupling behavior and dissipation functions are derived.

Next, the full model is simplified to a set of one-dimensional model problems: pure shear loading and pure longitudinal compression. These two formulations comprise the extremes of one-dimensional behavior and can be examined as simplified models of physical behavior of interest. The shear loading problem is a simplified model of shear-banding and localization phenomena while the longitudinal problem is a model of shock compression such as might be seen in a flyer-plate experiment. These problems are solved numerically using essentially non-oscillatory (ENO) and total variation diminishing (TVD) methods. The solutions reveal extremely rich behavior including complex wave phenomena, strain localization, and changes of material phase.